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| | | | |
|--------------|----|------------|---|
| NEWS | 1 | | Web Page for STN Seminar Schedule - N. America |
| NEWS | 2 | MAR 15 | WPIDS/WPIX enhanced with new FRAGHITSTR display format |
| NEWS | 3 | MAR 16 | CASREACT coverage extended |
| NEWS | 4 | MAR 20 | MARPAT now updated daily |
| NEWS | 5 | MAR 22 | LWPI reloaded |
| NEWS | 6 | MAR 30 | RDISCLOSURE reloaded with enhancements |
| NEWS | 7 | APR 02 | JICST-EPLUS removed from database clusters and STN |
| NEWS | 8 | APR 30 | GENBANK reloaded and enhanced with Genome Project ID field |
| NEWS | 9 | APR 30 | CHEMCATS enhanced with 1.2 million new records |
| NEWS | 10 | APR 30 | CA/CAPplus enhanced with 1870-1889 U.S. patent records |
| NEWS | 11 | APR 30 | INPADOC replaced by INPADOCDB on STN |
| NEWS | 12 | MAY 01 | New CAS web site launched |
| NEWS | 13 | MAY 08 | CA/CAPplus Indian patent publication number format defined |
| NEWS | 14 | MAY 14 | RDISCLOSURE on STN Easy enhanced with new search and display fields |
| NEWS | 15 | MAY 21 | BIOSIS reloaded and enhanced with archival data |
| NEWS | 16 | MAY 21 | TOXCENTER enhanced with BIOSIS reload |
| NEWS | 17 | MAY 21 | CA/CAPplus enhanced with additional kind codes for German patents |
| NEWS | 18 | MAY 22 | CA/CAPplus enhanced with IPC reclassification in Japanese patents |
| NEWS | 19 | JUN 27 | CA/CAPplus enhanced with pre-1967 CAS Registry Numbers |
| NEWS | 20 | JUN 29 | STN Viewer now available |
| NEWS | 21 | JUN 29 | STN Express, Version 8.2, now available |
| NEWS | 22 | JUL 02 | LEMBASE coverage updated |
| NEWS | 23 | JUL 02 | LMEDLINE coverage updated |
| NEWS | 24 | JUL 02 | SCISEARCH enhanced with complete author names |
| NEWS | 25 | JUL 02 | CHEMCATS accession numbers revised |
| NEWS | 26 | JUL 02 | CA/CAPplus enhanced with utility model patents from China |
| NEWS | 27 | JUL 16 | CAPplus enhanced with French and German abstracts |
| NEWS EXPRESS | 29 | JUNE 2007: | CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007. |
| NEWS HOURS | | | STN Operating Hours Plus Help Desk Availability |
| NEWS LOGIN | | | Welcome Banner and News Items |
| NEWS IPC8 | | | For general information regarding STN implementation of IPC 8 |

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***** STN Columbus *****

FILE 'HOME' ENTERED AT 16:26:46 ON 17 JUL 2007

=> file registry

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 16:26:54 ON 17 JUL 2007

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STRUCTURE FILE UPDATES: 16 JUL 2007 HIGHEST RN 942468-13-5

DICTIONARY FILE UPDATES: 16 JUL 2007 HIGHEST RN 942468-13-5

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

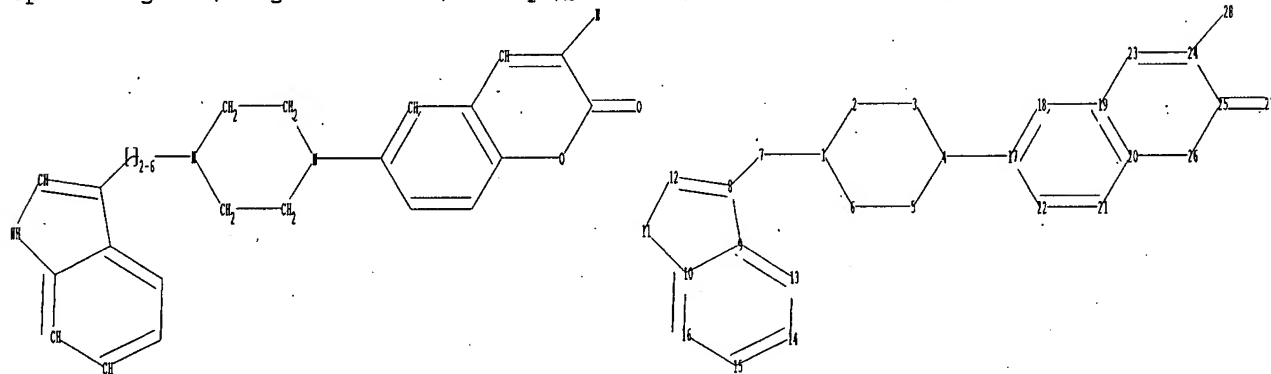
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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10 series\10551997\10551997b.str



chain nodes :

7 27 28

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
25 26

chain bonds :

1-7 4-17 7-8 24-28 25-27

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 9-13 10-11 10-16 11-12 13-14
 14-15 15-16 17-18 17-22 18-19 19-20 19-23 20-21 20-26 21-22 23-24 24-25
 25-26
 exact/norm bonds :
 1-7 4-17 10-11 11-12 24-28 25-27
 exact bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 7-8 8-9 8-12 19-23 20-26 23-24 24-25 25-26
 normalized bonds :
 9-10 9-13 10-16 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22
 isolated ring systems :
 containing 1 : 8 : 17 :

Match level :

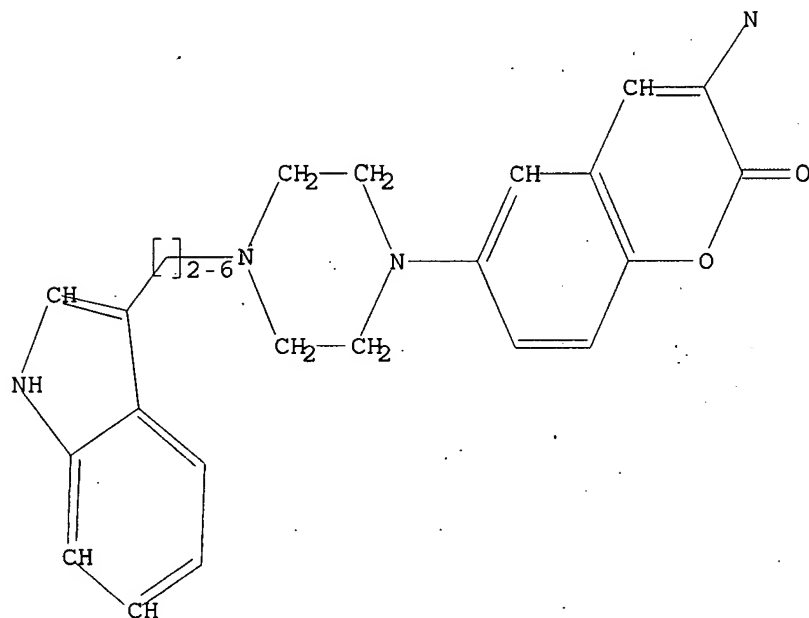
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 16:27:14 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED

0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 16:27:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED 45 TO ITERATE

100.0% PROCESSED 45 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

L3 8 SEA SSS FUL L1

=> file caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 172.10 | 172.31 |

FILE 'CAPLUS' ENTERED AT 16:27:23 ON 17 JUL 2007
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FILE LAST UPDATED: 16 Jul 2007 (20070716/ED)

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=> s l3

L4 2 L3

=> d l4 1-2 ibib abs hitstr

ACCESSION NUMBER: 2004:141760 CAPLUS

DOCUMENT NUMBER: 141:350194

TITLE: Preparation of chromenonindole derivatives as 5-HTX agonists and/or antagonists
 INVENTOR(S): Schiemann, Kai; Boettcher, Henning; Heinrich, Timo; Hoelzemann, Guenter; Van Amsterdam, Christoph; Bartoszyk, Gerd; Leibrock, Jochim; Seyfried, Christoph

PATENT ASSIGNEE(S): Merck Patent GmbH, Germany

SOURCE: Ger. Offen., 19 pp.

CODEN: GWXXBX

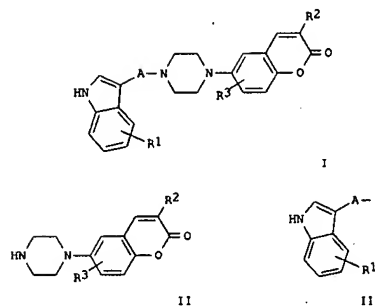
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|------------------|----------|
| DE 10315285 | A1 | 20041014 | DE 2003-10315285 | 20030404 |
| AU 2004226279 | A1 | 20041014 | AU 2004-226279 | 20040308 |
| CA 2520892 | A1 | 20041014 | CA 2004-2520892 | 20040308 |
| WO 2004087692 | A1 | 20041014 | WO 2004-EP2351 | 20040308 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1611126 | A1 | 20060104 | EP 2004-718300 | 20040308 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK | | | | |
| BR 2004008467 | A | 20060404 | BR 2004-8467 | 20040308 |
| CN 1768056 | A | 20060503 | CN 2004-80008571 | 20040308 |
| JP 2006522034 | T | 20060928 | JP 2006-504582 | 20040308 |
| US 20065258680 | A1 | 20061116 | US 2005-551997 | 20051004 |
| PRIORITY APPLN. INFO.: DE 2003-10315285 A 20030404 | | | | |
| WO 2004-EP2351 W 20040308 | | | | |
| OTHER SOURCE(S): CASREACT 141:350194; MARPAT 141:350194 | | | | |
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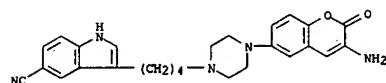


AB Chromenone-indole derivs. I [R1 = H, OH, CN, halogen, CONHR, OB, CO2B, CF3, NO2, NR2, NRCOR, NRCO2R, NRCONR2; R2 = NR2, NRCOR, NRCO2R, NRCONR2, NO2, NR5O2R, NRCSB, NRCSNR2; R3 = H, OH, CN, halogen, CONHR, OB, CO2B, CF3, NO2, NR2, NRCOR, NRCO2R, NRCONR2; R = H, B, Het, Ar; A = (unbranched, unsatd. C2-6-alkyl; S = (un)branched C1-6-alkyl], as well as of them pharmaceutical usable prodrugs, derivs., solvates, stereoisomers and salts show special effects on the central nervous system, above all 5-HT reabsorption inhibiting and 5-HTX agonistic and/or antagonistic effects. The procedure for the preparation of I is characterized by: alkylation of piperazine II by indole derivative III [L = Cl, Br, I, OH]. Thus, EMD 391987 [I·HCl; A = (CH2)4, R1 = CN-5, R2 = NHAc, R3 = H], was prepared from piperazine II [R2 = NHAc, R3 = H] via N-alkylation with indole III [A = (CH2)4, R1 = CN-5, L = I] in N-methylpyrrolidone containing EtN(CPh)2, followed by treatment with HCl. They are characterized by a particularly high bioavailability and a particularly high inhibition of the 5 HT reabsorption (see graphs).

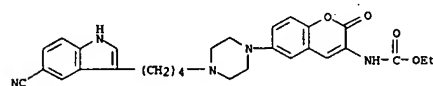
IT 752258-06-3P, EMD 480246 752258-08-5P
 752258-10-9P, EMD 391987 752258-11-0P, EMD 487535
 773878-58-3P 774242-09-0P, EMD 480247
 774242-10-3P, EMD 480248
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of chromenonindole derivs. as 5-HTX agonists and/or antagonists)

RN 752258-06-3 CAPLUS
 CN 1H-Indole-5-carbonitrile, 3-[4-[4-(5-amino-2-oxo-2H-1-benzopyran-6-yl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)

(Continued)

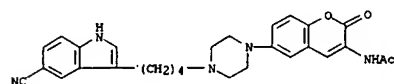


RN 752258-08-5 CAPLUS
 CN Carbamic acid, [6-[4-[4-(5-cyano-1H-indol-3-yl)butyl]-1-piperazinyl]-2-oxo-2H-1-benzopyran-3-yl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



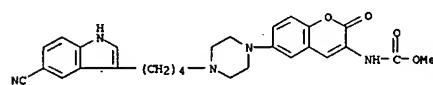
● HCl

RN 752258-10-9 CAPLUS
 CN Acetamide, N-[6-[4-[4-(5-cyano-1H-indol-3-yl)butyl]-1-piperazinyl]-2-oxo-2H-1-benzopyran-3-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



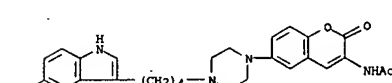
● HCl

RN 752258-11-0 CAPLUS
 CN Carbamic acid, [6-[4-[4-(5-cyano-1H-indol-3-yl)butyl]-1-piperazinyl]-2-oxo-2H-1-benzopyran-3-yl]-, methyl ester (9CI) (CA INDEX NAME)

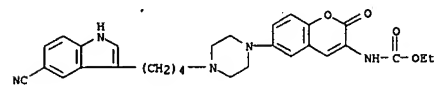


RN 773878-58-3 CAPLUS
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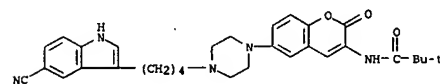
(Continued)



RN 774242-09-0 CAPLUS
 CN Carbamic acid, [6-[4-[4-(5-cyano-1H-indol-3-yl)butyl]-1-piperazinyl]-2-oxo-2H-1-benzopyran-3-yl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 774242-10-3 CAPLUS
 CN Propanamide, N-[6-[4-[4-(5-cyano-1H-indol-3-yl)butyl]-1-piperazinyl]-2-oxo-2H-1-benzopyran-3-yl]-2,2-dimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:710478 CAPLUS

DOCUMENT NUMBER: 141:235678

TITLE: Dual 5-HT1A agonists and 5-HT re-uptake inhibitors by combination of indole-butyl-amine and chromenonyl-piperazine structural elements in a single molecular entity

AUTHOR(S): Heinrich, Timo; Boettcher, Henning; Schiemann, Kai; Hoelzemann, Guenter; Schwarz, Michael; Bartoszyk, Gerd D.; van Amsterdam, Christoph; Greiner, Hartmut E.; Seyfried, Christoph A.

CORPORATE SOURCE: APReclinical Pharmaceutical Research, Merck KGaA, Darmstadt, 64293, Germany

SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(18), 4843-4852

CODEN: BMECEP; ISSN: 0958-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:235678

AB The dual serotonin (5-HT) re-uptake inhibitor and 5-HT1A receptor agonist vilazodone was found to increase central serotonin levels in rat brain. In the course of structural modifications of vilazodone 3-[4-{4-(2-oxo-2H-1-benzopyran-6-yl)-1-piperazinyl}-butyl]-1H-indole-5-carbonitrile and its fluorine analog 6-[4-{4-(5-fluor-3-indolyl)-butyl]-1-piperazinyl]-2H-1-benzopyran-2-one have been identified. These unsubstituted chromenones are equally potent at the 5-HT1A receptor and 5-HT transporter. The implementation of nitrogen functionalities in position 3 of the chromenones resulted in compds. acting as agonists at the 5-HT1A receptor and as 5-HT re-uptake inhibitors like vilazodone. Ex vivo 5-HT re-uptake inhibition and in vitro 5-HT agonism were determined in

the PCA- and GTPyS-assay, resp. The potential of these chromenones to increase central 5-HT levels was measured in microdialysis studies and especially the derive.

3-[4-{4-(3-amino-2-oxo-2H-chromen-6-yl)-piperazin-1-yl}-butyl]-1H-indole-5-carbonitrile, Et 6-[4-{4-(5-cyano-1H-indol-3-yl)-butyl]-piperazin-1-yl]-2-oxo-2H-chromen-3-yl]-carbamate and N-[6-[4-{4-(5-cyano-1H-indol-3-yl)-butyl]-piperazin-1-yl]-2-oxo-2H-chromen-3-yl]-acetamide give rise to rapid development of increased serotonin levels in rat brain cortex, lasting longer than 3 h.

IT 752258-06-3P 752258-07-4P 752258-08-5P

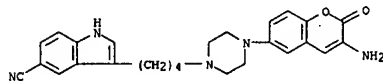
752258-10-9P 752258-11-0P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(dual 5-HT1A agonists and 5-HT re-uptake inhibitors by combination of indole-Bu-amine and chromenonyl-piperazine structural elements in a single mol. entity)

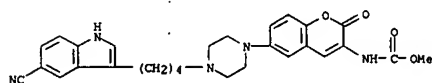
RN 752258-06-3 CAPLUS

CN 1H-Indole-5-carbonitrile, 3-[4-{4-(3-amino-2-oxo-2H-1-benzopyran-6-yl)-1-piperazinyl}butyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)



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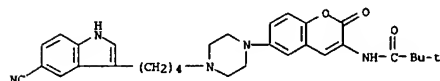
32

THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 752258-07-4 CAPLUS

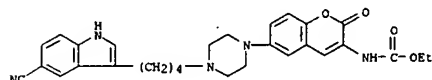
CN Propanamide, N-[6-[4-{4-(5-cyano-1H-indol-3-yl)butyl]-1-piperazinyl]-2-oxo-2H-1-benzopyran-3-yl]-2,2-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 752258-08-5 CAPLUS

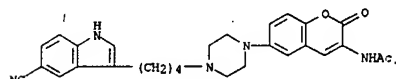
CN Carbamic acid, [6-[4-{4-(5-cyano-1H-indol-3-yl)butyl]-1-piperazinyl]-2-oxo-2H-1-benzopyran-3-yl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 752258-10-9 CAPLUS

CN Acetamide, N-[6-[4-{4-(5-cyano-1H-indol-3-yl)butyl]-1-piperazinyl]-2-oxo-2H-1-benzopyran-3-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 752258-11-0 CAPLUS

CN Carbamic acid, [6-[4-{4-(5-cyano-1H-indol-3-yl)butyl]-1-piperazinyl]-2-oxo-2H-1-benzopyran-3-yl]-, methyl ester (9CI) (CA INDEX NAME)

=> d his

(FILE 'HOME' ENTERED AT 16:26:46 ON 17 JUL 2007)

FILE 'REGISTRY' ENTERED AT 16:26:54 ON 17 JUL 2007

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 8 S L1 FULL

FILE 'CAPLUS' ENTERED AT 16:27:23 ON 17 JUL 2007

L4 2 S L3

=> log y

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

13.36

185.67

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY

TOTAL
SESSION

CA SUBSCRIBER PRICE

-1.56

-1.56

STN INTERNATIONAL LOGOFF AT 16:30:59 ON 17 JUL 2007

EAST Search History

| Ref # | Hits | Search Query | DBs | Default Operator | Plurals | Time Stamp |
|-------|------|----------------------|--|------------------|---------|------------------|
| L2 | 524 | 514/254.09.ccls. | US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB | OR | ON | 2007/07/17 17:21 |
| L3 | 1 | chromenoneindole | US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB | AND | ON | 2007/07/17 17:22 |
| L4 | 1 | l2 l3 | US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB | AND | ON | 2007/07/17 17:23 |
| L5 | 111 | l2 dopamine | US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB | AND | ON | 2007/07/17 17:23 |
| L6 | 107 | l2 dopamine receptor | US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB | AND | ON | 2007/07/17 17:24 |
| L7 | 54 | l2 serotonin uptake | US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB | AND | ON | 2007/07/17 17:24 |
| S2 | 2 | "7084143".pn. | US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB | OR | ON | 2007/07/17 11:39 |

EAST Search History

| | | | | | | |
|----|---|---------------|--|----|----|------------------|
| S3 | 2 | "4376123".pn. | US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB | OR | ON | 2007/07/17 17:21 |
|----|---|---------------|--|----|----|------------------|